

# Simulations of Radiative Transfer in Combustion Systems and Further Developments of High-Order Spherical Harmonics Methods

Wenjun Ge

Department of Mechanical Engineering  
School of Engineering  
University of California, Merced  
Merced, CA 95343, USA

*wge@ucmerced.edu*



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- 1 Introduction
- 2 Spectral Models and FSK Look-Up Table
- 3 RTE Solvers and Spherical Harmonics ( $P_N$ ) Methods
- 4 Gray Examples
- 5 Applications in Combustion Simulations

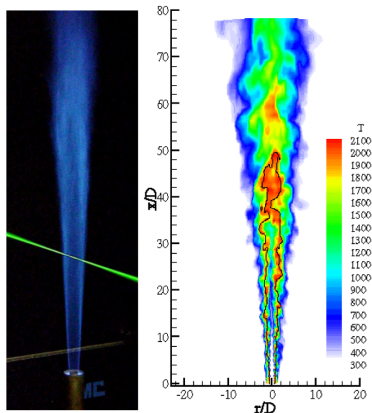
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# Combustion and combustion simulations

- Combustion is a chemical process in which a fuel reacts rapidly with oxygen and gives off heat.
- High-fidelity simulations: chemistry, turbulence, radiation and their interactions.



Source: left from SpaceX, top-right from internet  
bottom-right from Imamori, Y. et al., 2011

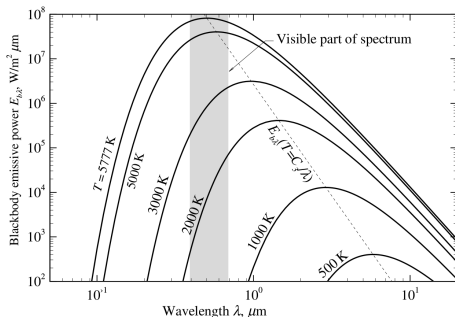


Source: left from Sandia NL, right from Pitsch, H., 2006



# Radiative transfer

- Radiative transfer → electromagnetic waves → **spectral dependence** and travelling at  $3 \times 10^8$  m/s in vacuum
- The radiative energy emitted by a blackbody is proportional to the fourth power of temperature → **importance in high-temperature applications, nonlinearity**
- Radiative transfer in participating/particulate media → emission, absorption and scattering → **directional dependence**



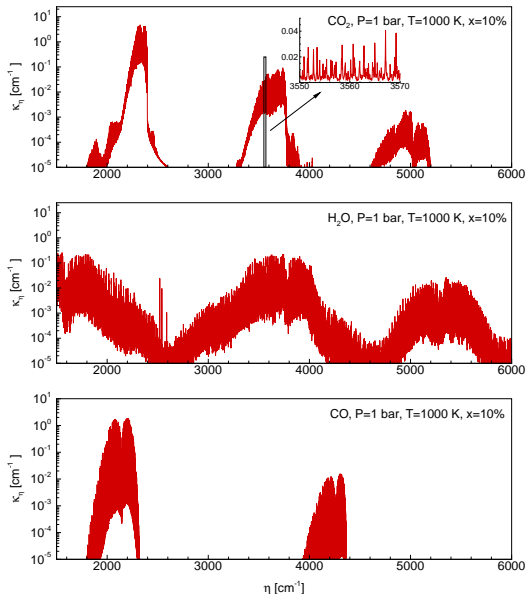
- $E_b(T) = \int E_{b,\lambda} d\lambda = n^2 \sigma_{SB} T^4.$

- Combustion problems generally involve temperature levels between **500 K** and **2800 K** so that the spectral ranges of interest in combustion applications are from  $0.7 \mu\text{m}$  to  $30 \mu\text{m}$  (or  $300 \sim 14000 \text{ cm}^{-1}$  in wavenumber).

Figure : Blackbody emissive power spectrum.

# Radiative properties of molecular gases

- Vibration-rotation bands from bound-bound transitions
- The broadening of the spectral lines due to collisions and Doppler effect
- Modern databases: HITEMP, HITRAN, CDSD.
- $\kappa_{\eta}(\mathbf{Y}, T, p)$



## Radiative transfer equation (RTE) and radiative heat source

Radiative transfer in an absorbing, emitting and scattering medium is formulated by considering conservation of radiative energy, known as the **radiative transfer equation** (RTE).

RTE:

$$\hat{\mathbf{s}} \cdot \nabla_{\tau} I_{\eta} + I_{\eta} = (1 - \omega_{\eta}) I_{b\eta} + \frac{\omega}{4\pi} \int_{4\pi} I_{\eta}(\hat{\mathbf{s}}') \Phi_{\eta}(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}') d\Omega'$$

The net energy balance at any location in the medium is obtained by integrating the spectral intensity over **all directions** and **all wavenumbers**. The **radiative heat source**  $S_{rad}$ , is the difference between local absorption and emission:

Radiative heat source:

$$S_{rad} = -\nabla \cdot \mathbf{q}_{rad} = -S_{emi} + S_{abs} = -4\kappa_P \sigma_{SB} T^4 + \int_0^{\infty} \kappa_{\eta} \int_{4\pi} I_{\eta}(\tau, \hat{\mathbf{s}}) d\Omega d\eta$$

# Coupling to the energy equation for turbulent reacting flows

DNS (direct numerical simulation):

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho h u_i}{\partial x_i} = -\frac{\partial J_i^h}{\partial x_i} + \frac{Dp}{Dt} + \tau_{ij} \frac{\partial u_j}{\partial x_i} + S_{rad}$$

LES (large eddy simulation):

$$\frac{\partial \bar{\rho} \tilde{h}}{\partial t} + \frac{\partial \bar{\rho} \tilde{h} \tilde{u}_i}{\partial x_i} = \frac{\partial (\bar{\rho} \tilde{h} \tilde{u}_i - \bar{\rho} \tilde{h} \tilde{u}_i)}{\partial x_i} - \frac{\partial \bar{J}_i^h}{\partial x_i} + \frac{D\bar{p}}{Dt} + \overline{\tau_{ij} \frac{u_j}{x_i}} + \overline{S_{rad}}$$

RANS (Raynolds-Averaged Navier-Stokes):

$$\frac{\partial \langle \rho \rangle \tilde{h}}{\partial t} + \frac{\partial \langle \rho \rangle \tilde{h} \tilde{u}_i}{\partial x_i} = \frac{\partial (\langle \rho \rangle \tilde{h} \tilde{u}_i - \langle \rho \rangle \tilde{h} \tilde{u}_i)}{\partial x_i} - \frac{\partial \langle J_i^h \rangle}{\partial x_i} + \frac{D\langle p \rangle}{Dt} + \langle \tau_{ij} \frac{u_j}{x_i} \rangle + \langle S_{rad} \rangle$$

# Turbulence-radiation interaction (TRI)

Time-averaged radiative source  $\langle S_{rad} \rangle$  accounting for turbulence effects:

$$\langle S_{rad} \rangle = -\langle S_{emi} \rangle + \langle S_{abs} \rangle = -4\pi\sigma_{SB}\langle\kappa_P I_b\rangle + \int_0^\infty \int_{4\pi} \langle\kappa_\eta I_\eta\rangle d\Omega d\eta$$

Emission TRI and absorption TRI:

$$\text{Emission TRI: } \langle\kappa_P I_b\rangle \neq \kappa_P(\langle\phi\rangle)I_b(\langle T\rangle)$$

$$\text{Absorption TRI: } \langle\kappa_\eta I_\eta\rangle \neq \kappa_\eta(\langle\phi\rangle)I_\eta(\langle\phi\rangle)$$

e.g. autocorrelation of  $I_b$ :

$$\mathcal{R}_{I_b} = \frac{I_b(\langle T \rangle)}{\langle I_b(T) \rangle} = \frac{(\langle T \rangle)^4}{\langle T^4 \rangle} \neq 1$$

# Interactions between radiation and reacting flow

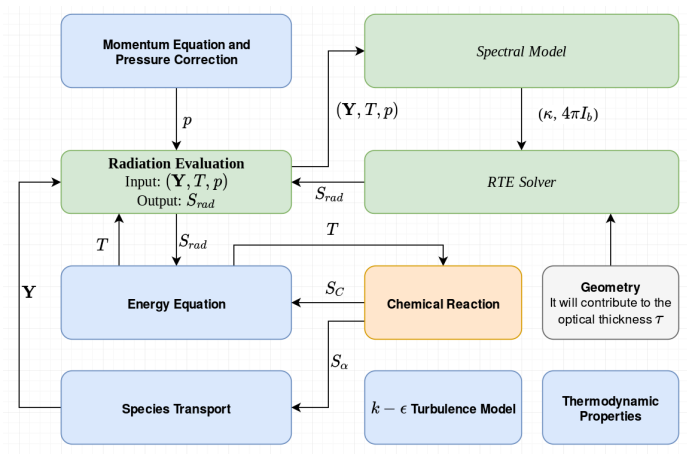


Figure : Schematic of the coupling between radiation and other sub-models

## Example: Sandia Flame D $\times$ 4 - RANS Simulation

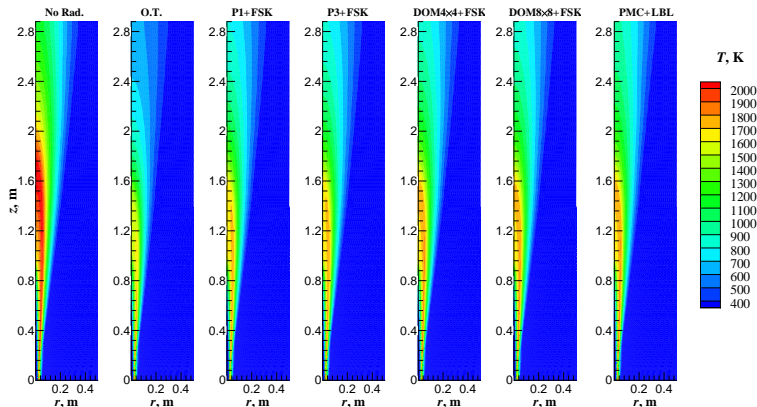
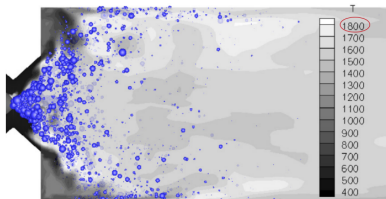


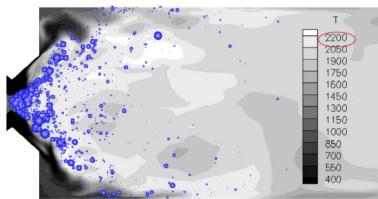
Figure : RANS Simulations of Sandia Flame D $\times$ 4

- Not considering radiation will **overpredict** the peak temperature by up to **300 K**
- Optically-thin model will **underpredict** the temperature about **200 K**

# Example: Aircraft Engine - LES Simulation

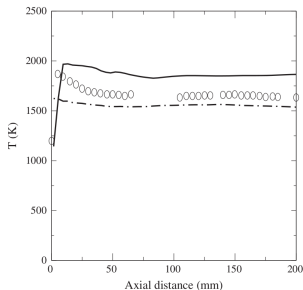


(a) With radiation



(b) No radiation

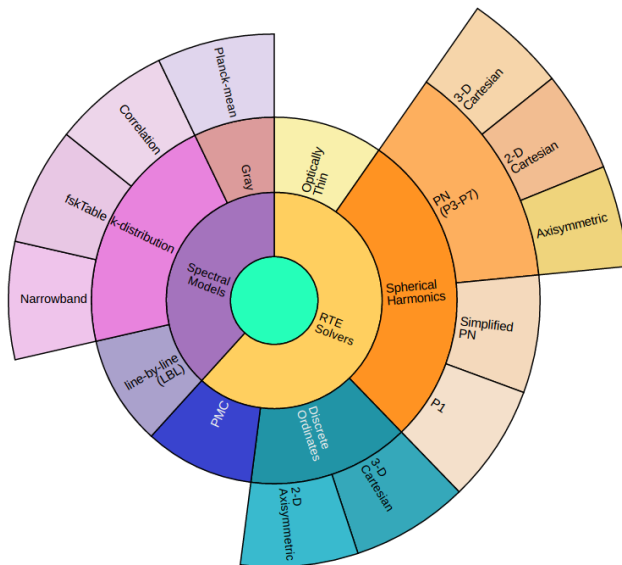
Figure : Droplet dist. sized by droplet mass and temp. dist. Source: CTR Stanford and NASA, 2014



- No Rad. v.s. O.T. (gas phase)
- $T_{peak}$  from O.T. is 400 K lower
- lower evaporation rates from O.T



# Nongray radiation module



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# Summary of spectral models

- Gray model (Planck-mean)
  - Weighted average over the entire spectrum
  - Cheap, but inaccurate; Underpredict the absorption
  - In practice: most popular
- Band models
  - Constant properties over narrow or wide bands
  - Case dependent accuracy
  - In practice: popular, becoming less popular
- Full-spectrum  $k$ -distribution (FSK) or similar models (WSGG)
  - Reordering reoccurring spectral absorption coefficients
  - Very accurate; implementation dependent
  - In practice: less popular, becoming more popular
- Line-by-line (LBL) Calculations
  - The most accurate
  - Only practical for stochastic solution methods (PMC)
  - In practice: becoming more popular with Monte Carlo solution method

## Gray model: constant absorption coefficient

Weighting the spectral absorption coefficient  $\kappa_\eta$  with the Planck function  $I_{b\eta}$ :

### Planck-mean absorption coefficient:

$$\kappa_P = \frac{\int_0^\infty \kappa_\eta I_{b\eta} d\eta}{\int_0^\infty I_{b\eta} d\eta} = \frac{\int_0^\infty \kappa_\eta I_{b\eta} d\eta}{\sigma_{SB} T^4}$$

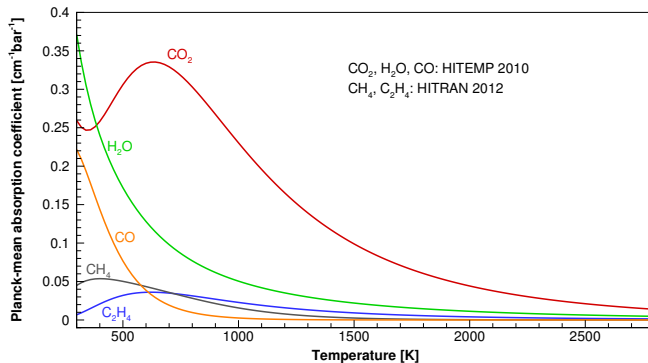
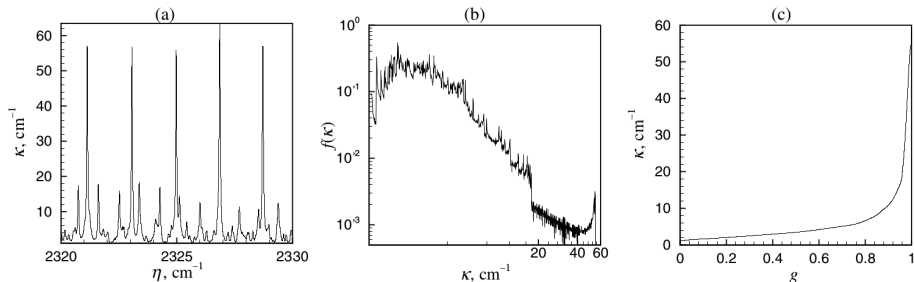


Figure : Planck-mean absorption coefficients of CO<sub>2</sub>, H<sub>2</sub>O, CO, CH<sub>4</sub> and C<sub>2</sub>H<sub>4</sub>

# Full-spectrum $k$ -distribution (FSK) model: reordering reoccurring $\kappa_\eta$

- Reduce the number of evaluations of the RTE required from 1 million to 8~16.



**Figure :** (a) Spectral absorption coefficient (b) PDF and (c)  $k$ -distribution for  $4.5 \mu\text{m}$   $\text{CO}_2$  band at  $T=1000 \text{ K}$  and  $p=1 \text{ bar}$ .

- 1  $\eta - \kappa_\eta$
- 2  $k - f(k)$ ,  $f(k)$  is a weighted sum of the number of points where  $\kappa_\eta = k$
- 3  $g - k$ ,  $g$  is the cumulative distribution function of  $f(k)$

# Comparison of different FSK implementations

- generate  $k$ -distributions for individual species
  - [Narrowband database](#) - very accurate, less memory, more runtime computing
  - [Correlations](#) - less accurate, less memory, less runtime computing
- generate  $k$ -distributions for the mixture
  - [Look-up table](#) - very accurate, more memory, less computing

[Table](#) : CPU time comparisons of generating 10,000 arbitrary  $k$ -distributions of mixtures.

Database	Mixing model	CPU Time (s)
Narrowband	Multiplication	1389.65
	MRmixing	5904.59
Correlations	Multiplication	0.41
	MRmixing	8.97
Look-up table	-	0.26

# FSK Table for nonhomogeneous mixtures

Table : Precalculated thermodynamic states of the FSK look-up table.

Parameters	Range	Values	Number of points
Species	CO <sub>2</sub> , H <sub>2</sub> O and CO		3
Pressure (total)	0.1 ~ 0.5 bar	Every 0.1 bar	34
	0.7 bar	0.7 bar	
	1.0 ~ 14.0 bar	Every 1.0 bar	
	15.0 ~ 80.0 bar	Every 5.0 bar	
Gas temperature	300~ 3000 K	Every 100 K	28
Reference temperature	300~ 3000 K	Every 100 K	28
Mole fraction of CO <sub>2</sub>	0.0 ~ 0.05	Every 0.01	10
	0.25 ~ 1.0	Every 0.25	
Mole fraction of H <sub>2</sub> O	0.0 ~ 0.05	Every 0.01	13
	0.1 ~ 0.2	Every 0.05	
	0.25 ~ 1.0	Evert 0.25	
Mole fraction of CO	0.0 ~ 0.5	{0.0, 0.01, 0.05, 0.1, 0.25, 0.5 }	6

- The size of the table is about 5 GB.
- Apply dynamic loading to reduce memory demand.
- The look-up table can be customized for specific needs.

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# Summary of RTE solvers

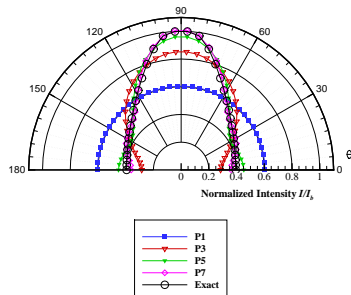
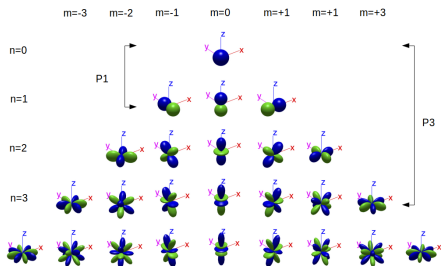
- Optically Thin (O.T.)
  - No absorption, only consider emission
  - Cheap, only useful for optically thin media
  - In practice: currently most popular
- Discrete Ordinates Method (DOM) or similar concepts
  - Discretize the angular profile of intensity by several finite directions
  - Cheap and accurate for non-scattering media, suffers from ray effects and false scattering for scattering media or reflecting surfaces
  - In practice: very popular, available in most commercial CFD softwares,  $DOM_{8 \times 8}$  is usually good enough
- Spherical Harmonics ( $P_N$ ) Method
  - Approximate the angular profile of intensity by a truncated series of spherical harmonics (a spectral method)
  - Very accurate for optically thick media; not accurate when intensity is directionally anisotropic
  - In practice:  $P_1$  is very popular, high-order  $P_N$  needs more research
- Photon Monte Carlo (PMC)
  - The most accurate and robust
  - Used to be considered impractical
  - In practice: becoming more and more popular

# Spherical harmonics ( $P_N$ ) method

Truncated series of spherical harmonics of order  $N$ :

$$I(\tau, \hat{\mathbf{s}}) = \sum_{n=0}^N \sum_{m=-n}^n I_n^m(\tau) Y_n^m(\hat{\mathbf{s}}), \quad Y_n^m(\psi, \theta) = \begin{cases} \cos(m\psi) P_n^m(\cos \theta) & \text{for } m \geq 0 \\ \sin(|m|\psi) P_n^m(\cos \theta) & \text{for } m < 0 \end{cases}$$

- Use spherical harmonics as bases for the angular profile of intensity
- Transform the RTE into equations of the intensity coefficients  $I_n^m$



# The 3-D formulation

## Governing equations

- Substitute the spherical harmonics series into the RTE;
- Multiply the resulting equation by  $Y_n^m$  and integrate the whole equation over a solid angle of  $4\pi$ ; One obtains  $(N + 1)^2$  first-order PDEs;
- The second-order elliptic formulation is obtained by eliminating the odd order intensity coefficients ( $I_n^m$  with odd  $n$ ) by their relation to the gradients of  $I_{n+1}^m$  and  $I_{n-1}^m$ ; This will reduce the number of governing equations to  $N(N + 1)/2$ .

Table : Intensity coefficients employed for 3-D Cartesian formulation

$n$	Intensity Coefficients												
0	$I_0^0$												
2	$I_2^{-2} \quad I_2^{-1} \quad I_2^0 \quad I_2^1 \quad I_2^2$												
4	$I_4^{-4} \quad I_4^{-3} \quad I_4^{-2} \quad I_4^{-1} \quad I_4^0 \quad I_4^1 \quad I_4^2 \quad I_4^3 \quad I_4^4$												
6	$I_6^{-6}$	$I_6^{-5}$	$I_6^{-4}$	$I_6^{-3}$	$I_6^{-2}$	$I_6^{-1}$	$I_6^0$	$I_6^1$	$I_6^2$	$I_6^3$	$I_6^4$	$I_6^5$	$I_6^6$
$n$	$I_n^{-n}$	$\dots$	$\dots$	$I_n^{-3}$	$I_n^{-2}$	$I_n^{-1}$	$I_n^0$	$I_n^1$	$I_n^2$	$I_n^3$	$\dots$	$\dots$	$I_n^n$

# Governing equations

For each  $Y_n^m : n = 0, 2, \dots, N-1, 0 \leq m \leq n$  :

$$\begin{aligned}
 & \sum_{k=1}^3 \left\{ (\mathcal{L}_{xx} - \mathcal{L}_{yy}) \left[ (1 + \delta_{m2}) a_k^{nm} I_{n+4-2k}^{m-2} + \frac{\delta_{m1}}{2} c_k^{nm} I_{n+4-2k}^m + e_k^{nm} I_{n+4-2k}^{m+2} \right] \right. \\
 & \quad + (\mathcal{L}_{xz} + \mathcal{L}_{zx}) \left[ (1 + \delta_{m1}) b_k^{nm} I_{n+4-2k}^{m-1} + d_k^{nm} I_{n+4-2k}^{m+1} \right] \\
 & \quad + (\mathcal{L}_{xy} + \mathcal{L}_{yx}) \left[ -(1 - \delta_{m2}) a_k^{nm} I_{n+4-2k}^{-(m-2)} + \frac{\delta_{m1}}{2} c_k^{nm} I_{n+4-2k}^{-m} + e_k^{nm} I_{n+4-2k}^{-(m+2)} \right] \\
 & \quad + (\mathcal{L}_{yz} + \mathcal{L}_{zy}) \left[ -(1 - \delta_{m1}) b_k^{nm} I_{n+4-2k}^{-(m-1)} + d_k^{nm} I_{n+4-2k}^{-(m+1)} \right] \\
 & \quad \left. + (\mathcal{L}_{xx} + \mathcal{L}_{yy} - 2\mathcal{L}_{zz}) c_k^{nm} I_{n+4-2k}^m \right\} \\
 & + [\mathcal{L}_{zz} - (1 - \omega \delta_{0n})] I_n^m = -(1 - \omega) I_b \delta_{0n} \\
 & \text{where the operators: } \mathcal{L}_{xy} = \frac{1}{\beta} \frac{\partial}{\partial x} \left( \frac{1}{\beta} \frac{\partial}{\partial y} \right)
 \end{aligned}$$

Each governing equation is characterized by the spherical harmonics  $Y_n^m$ .

# Marshak's boundary conditions

For each  $\bar{Y}_{2i-1}^{\pm m}$ ,  $i = 1, 2, \dots, (N+1)/2$ :

$$\begin{aligned}
 0 = & \sum_{l=0}^{\frac{N-1}{2}} \sum_{m'=-2l}^{2l} p_{2l,2i-1}^m \bar{\Delta}_{\pm m, m'}^{2l} I_{2l}^{m'} \\
 & - \frac{\partial}{\partial \tau_{\bar{x}}} \sum_{l=l_1}^{\frac{N-1}{2}} \sum_{m'=-2l}^{2l} \left[ (1 \pm \delta_{m,1}) u_{l,i}^m \bar{\Delta}_{\pm(m-1), m'}^{2l} - v_{l,i}^m \bar{\Delta}_{\pm(m+1), m'}^{2l} \right] I_{2l}^{m'} \\
 & \pm \frac{\partial}{\partial \tau_{\bar{y}}} \sum_{l=l_2}^{\frac{N-1}{2}} \sum_{m'=-2l}^{2l} \left[ (1 \mp \delta_{m,1}) u_{l,i}^m \bar{\Delta}_{\mp(m-1), m'}^{2l} + v_{l,i}^m \bar{\Delta}_{\mp(m+1), m'}^{2l} \right] I_{2l}^{m'} \\
 & - \frac{\partial}{\partial \tau_{\bar{z}}} \sum_{l=0}^{\frac{N-1}{2}} \sum_{m'=-2l}^{2l} w_{l,i}^m \bar{\Delta}_{\pm m, m'}^{2l} I_{2l}^{m'}
 \end{aligned}$$

Each boundary condition is characterized by the local spherical harmonics  $\bar{Y}_{2i-1}^m$ .

## 2-D axisymmetric formulation

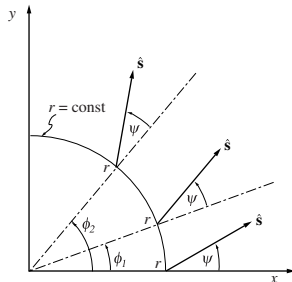
$I$  varies with  $r$  and axially with  $z$ , but not azimuthally with  $\phi$

$$I(r, \phi, z; \theta, \psi + \phi) = I(r, 0, z; \theta, \psi)$$

$$I_n^m(r, \phi, z) = I_n^m(r, 0, z) \cos m\phi = \hat{I}_n^m \cos m\phi$$

$$I_n^{-m}(r, \phi, z) = I_n^m(r, 0, z) \sin m\phi = \hat{I}_n^m \sin m\phi$$

Employing the above relations to the general 3-D formulation, the number of governing equations is reduced to  $(N + 1)^2/4$  for axisymmetric geometry.

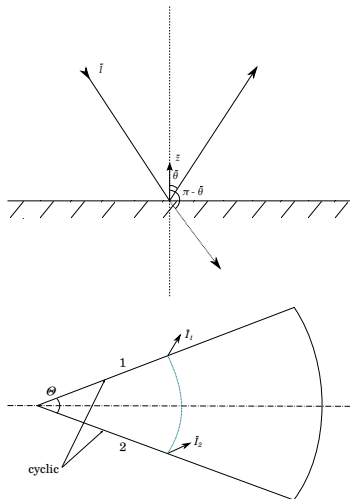


**Table :** Intensity coefficients employed for 2-D axisymmetric formulation

$n$	Intensity Coefficients						
0	$\hat{I}_0^0$						
2	$\hat{I}_2^0$	$\hat{I}_2^1$	$\hat{I}_2^2$				
4	$\hat{I}_4^0$	$\hat{I}_4^1$	$\hat{I}_4^2$	$\hat{I}_4^3$	$\hat{I}_4^4$		
6	$\hat{I}_6^0$	$\hat{I}_6^1$	$\hat{I}_6^2$	$\hat{I}_6^3$	$\hat{I}_6^4$	$\hat{I}_6^5$	$\hat{I}_6^6$
$n$	$\hat{I}_n^0$	$\hat{I}_n^1$	$\hat{I}_n^2$	$\hat{I}_n^3$	...	...	$\hat{I}_n^6$

# Development of special boundary conditions

- Specified radiative flux at the wall;
- Symmetry/specular reflection boundaries;
- Mixed diffuse-specular reflection surfaces;
- Cyclic boundaries.

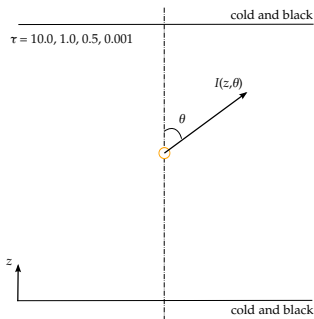


- Implementation platform → OpenFOAM® 2.2.x
- The spatial discretization → standard second-order finite volume method
- Solution method → segregated iterative method
- Solution of each governing equation (inner iterations) → the incomplete Cholesky preconditioned conjugated gradient method (PCG)
- Resolving the coupling between governing equations and Robin-type BCs (outer iterations) → Gauss Seidel method



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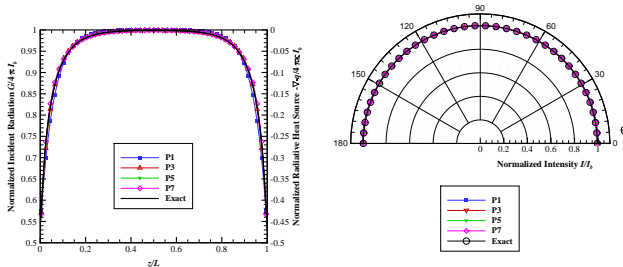
## Problem 1: 1-D slab with homogeneous radiative properties



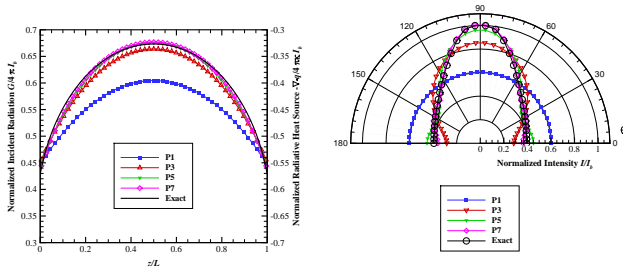
- 1-D Cartesian examples represent the radiative transfer between two infinitely long parallel plates;
- Geometry: 1-D Slab ( $1 \times 1 \times 101$ );
- All properties are normalized so that the only difference is the optical thickness;
- $-\nabla \cdot \mathbf{q}$  and  $G$  from  $P_1$  to  $P_7$  are compared to exact solution;
- Intensity  $I$  is reconstructed at the center ( $z/L = 0.5$ ) and is also compared with the exact intensity.

# Results of $\tau=10.0$ and $\tau=1.0$

$\tau=10$  (Optically thick):

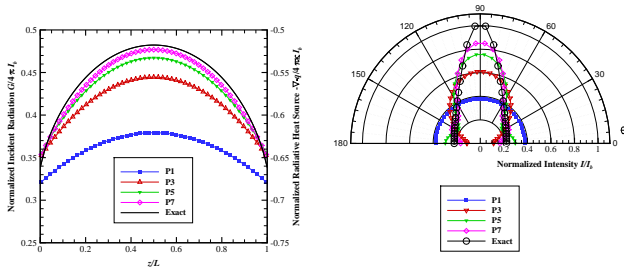


$\tau=1$ : (Optically intermediate):

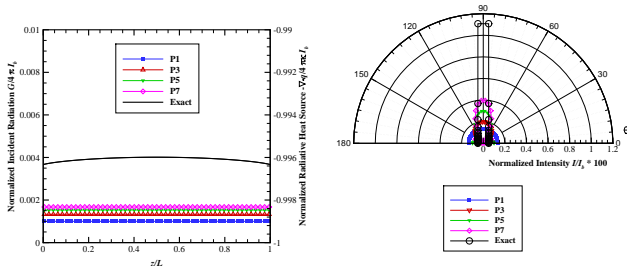


# Results of $\tau=0.5$ and $\tau=0.001$

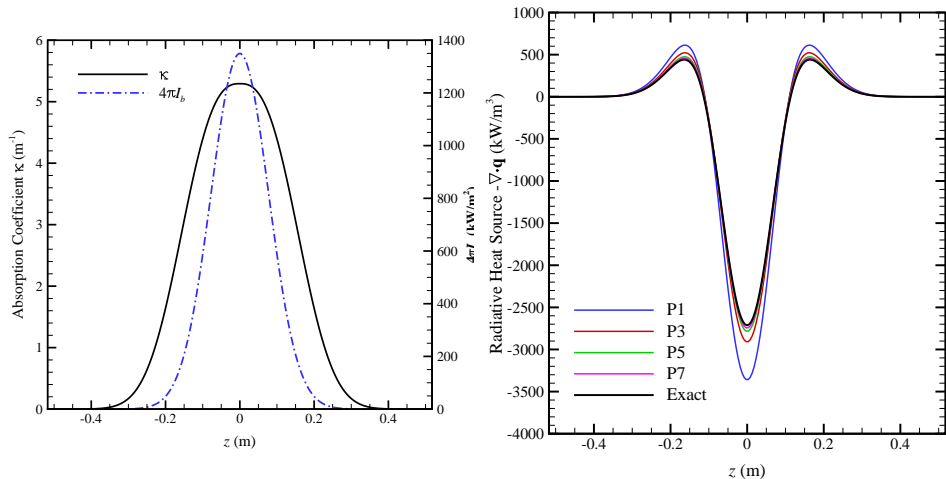
$\tau=0.5$  (Optically intermediate):



$\tau=0.001$  (Optically thin):



## Problem 2: 1-D slab with flame-like variable radiative properties



Geometry: 1-D Slab (200 cells),  $L=0.52 \times 2$  m;

# Rotational invariance and comparison with PMC

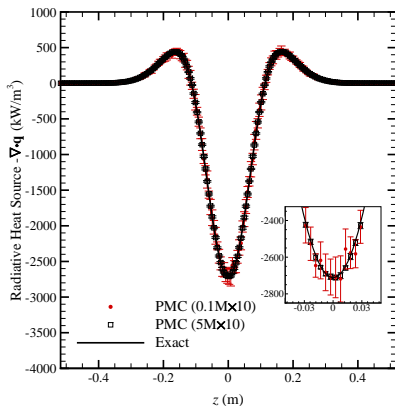
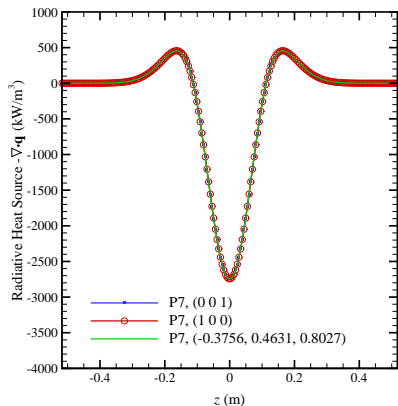


Table : Comparison of CPU time (s)

Num. of cells	$\tau_L$	$P_1$	$P_3$	$P_5$	$P_7$	PMC (0.1M×10)	PMC (5M×10)
200	0.886	0.01	0.10	0.52	1.34	45.7	2532.1

# Problem 3: 2-D square geometry

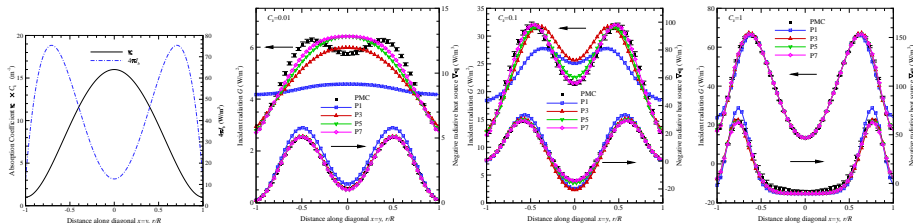


Table : Comparison of CPU time (s)

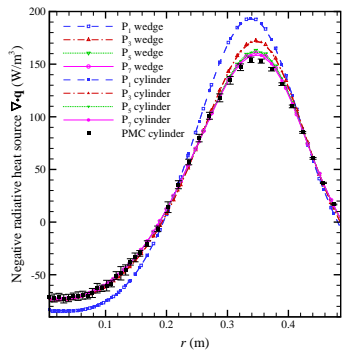
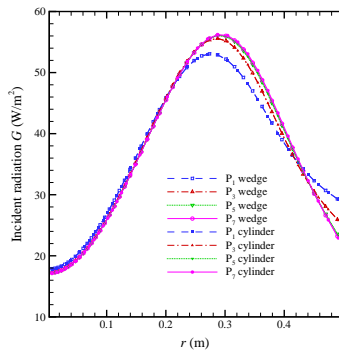
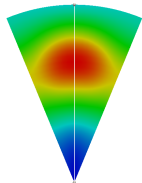
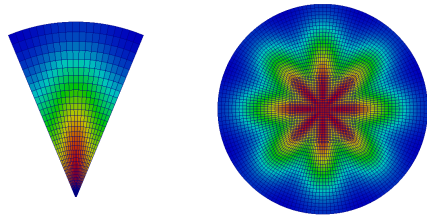
No. of cells	$C_k$	$\tau_R$	$P_1$	$P_3$	$P_5$	$P_7$	PMC
2,601 (51×51)	$C_k=1$	12.7	0.02	0.75	4.71	7.0	459 (5M×10)
	$C_k=0.1$	1.27	0.02	0.87	5.05	9.33	125.5 (0.5M×10)
	$C_k=0.01$	0.127	0.02	1.78	7.09	19.2	21.2 (0.05M×10)

# Problem 4: A 45-degree wedge and a full cylinder

$$I_b = 1 + \frac{20}{R^4} r^2 (R^2 - r^2) \quad \text{W} \cdot \text{m}^{-3}$$

$$\kappa = \left[ 1 + \frac{15}{R^4} (R^2 - r^2)^2 \right] \left( 1 + 0.5 \frac{r}{R} \cos 8\theta \right), \quad \text{m}^{-1}$$

$$0 \leq r \leq R = 0.5, \quad \text{m}$$





- 1 Introduction
- 2 Spectral Models and FSK Look-Up Table
- 3 RTE Solvers and Spherical Harmonics ( $P_N$ ) Methods
- 4 Gray Examples
- 5 Applications in Combustion Simulations**

# Coupled RANS Simulation - Sandia Flame D $\times$ 4

- Sandia Flame D is a turbulent piloted jet flame with a Reynolds number of  $Re_D=22,400$
- Fuel: Methane
- Diameter of main jet:  $d_j=7.2$  mm
- The flame is scaled up to show radiation effects.

	Sandia Flame D		Sandia Flame D $\times$ 4	
	$d$ (mm)	$u$ (m/s)	$d$ (mm)	$u$ (m/s)
main jet	7.2	49.89	28.8	12.4725
pilot	18.864	10.57	75.456	2.6425
co-flow	258.2	0.90	1032.8	0.2250

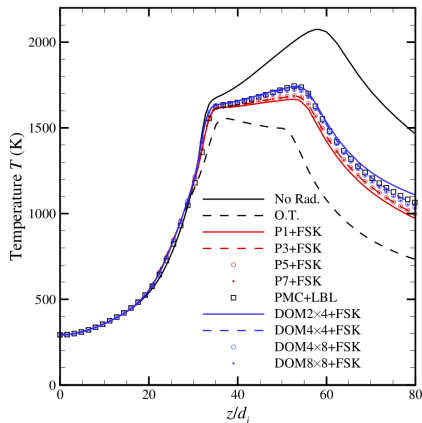
- Chemistry model: GRI-Mech 2.11 (49 species and 277 reactions), PaSR (partially-stirred reactor)
- Turbulence model: Standard two-equation  $k-\epsilon$  model
- Radiation models: O.T., PN+FSK, DOM+FSK, PMC+LBL



Source: Sandia NL

# Temperature profiles along the axis - Sandia Flame D×4

Temperature profiles along the axis after the flame reaches steady state:



Radiation Solvers	$T_{p,c}$ (K)	$\Delta T_{p,c}$ (K)
No Rad.	2074	/
O.T.	1554	-520
P1+FSK	1666	-408
P3+FSK	1683	-391
P5+FSK	1688	-386
P7+FSK	1689	-385
DOM 2×4	1744	-330
DOM 4×4	1736	-338
DOM 8×8	1721	-353
PMC+LBL	1745	-329

- Adding radiation models cools down the flame and results in around 3% less-complete combustion.
- Nearly 30% of the combustion heat release is transferred to the environment through radiation.

# Computational cost

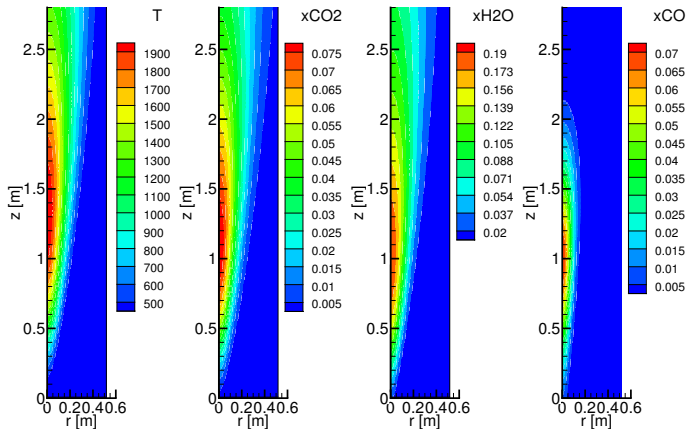
**Table :** Average CPU time per time step (radiation is evaluated once per 1/10/100/250 time steps for the PN/DOM+FSK solvers and the average  $t_{RTE} + t_{overhead}$  and  $t_{FSK}$  are only shown for runs with radiation evaluated once per time step)

Radiation Solver	Average CPU Time (s)	$t_{RTE}+t_{overhead}$ (s)	$t_{FSK}$ (s)	
No Rad	0.82	/	/	
P1+FSK	0.97/0.85/0.82/0.82	0.09	0.06	1 second-order PDE
P3+FSK	1.05/0.87/0.83/0.83	0.17		4 second-order PDE
P5+FSK	1.36/0.88/0.84/0.84	0.48		9 second-order PDE
P7+FSK	1.64/0.90/0.85/0.85	0.76		16 second-order PDE
DOM 2×4+FSK	1.11/0.86/0.85/0.84	0.23		8 first-order PDE
DOM 4×4+FSK	1.20/0.87/0.85/0.84	0.32		16 first-order PDE
DOM 4×8+FSK	1.42/0.91/0.86/0.86	0.54		32 first-order PDE
DOM 8×8+FSK	1.78/0.94/0.87/0.87	0.9		64 first-order PDE
PMC+LBL	0.87	0.05	/	5,000 with time-blending
PMC+LBL	0.92	0.10	/	10,000 with time-blending

All computations are performed on twelve 2.66 GHz Intel Xeon X7460 processors.

# Sandia Flame D×4, a frozen snapshot study

A mixture of hot  $\text{CO}_2$ ,  $\text{H}_2\text{O}$  and  $\text{CO}$ :

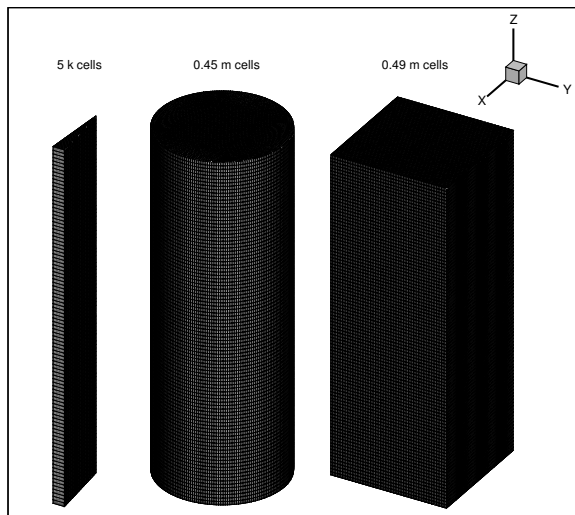


Spectral model for  $P_N$  and DOM: FSK-Table with eight quadrature points

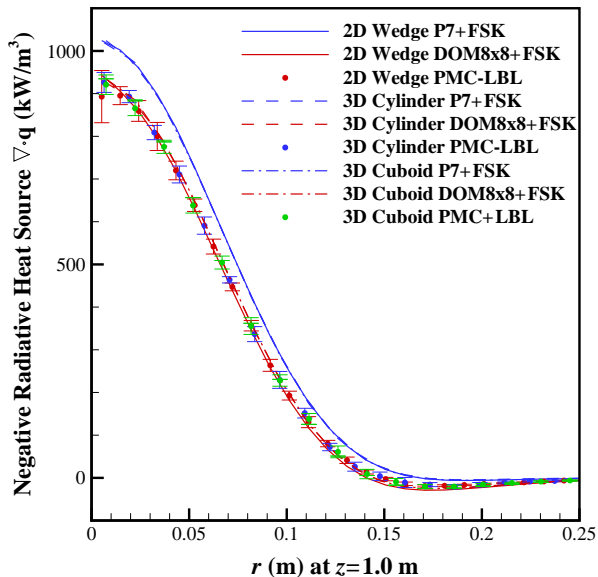
Spectral model for for PMC: LBL

# Grids

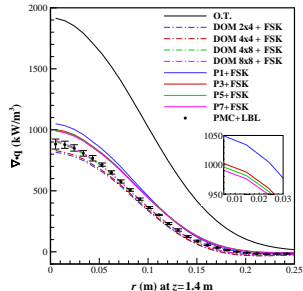
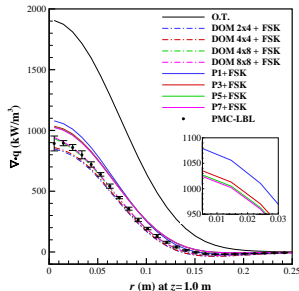
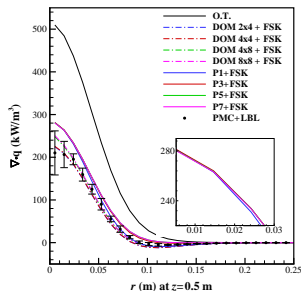
- Radiative calculations are conducted on a 2-D wedge, a 3-D cylinder and a 3-D cuboid
- The same axisymmetric distributions of temperature and mole fractions



## Results from different meshes



# Negative radiative heat source $\nabla \cdot \mathbf{q}$ from different RTEs

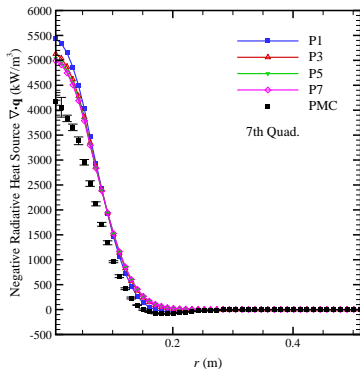
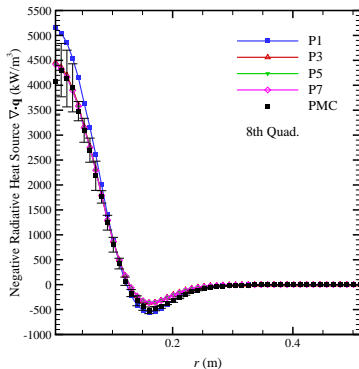




# The most important quadratures

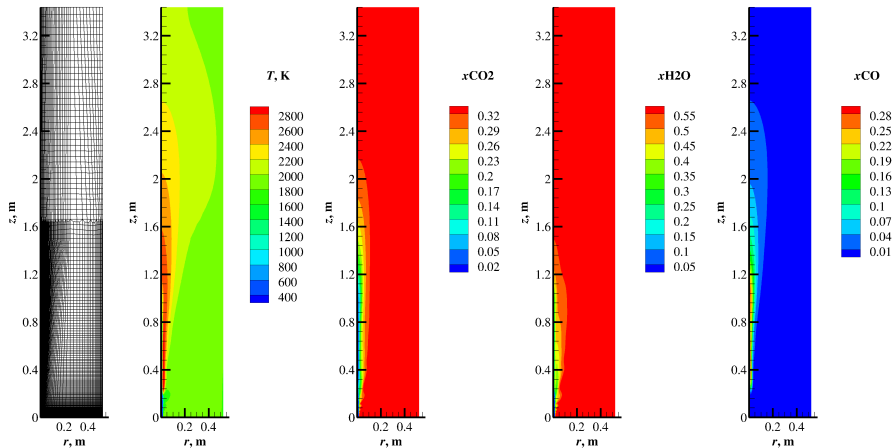
Table : Optical thickness  $\tau_{R,g}$  along radius at  $z = 1.0$  m for each quadrature point

Index	1	2	3	4	5	6	7	8
$\tau_{R,g}$	0.0006	0.0035	0.0120	0.03348	0.08081	0.2112	0.8327	3.5118



# High-temperature oxy-natural gas flame

Oxy-fuel combustion is the process of burning a fuel using pure oxygen instead of air as the primary oxidant. A 0.8 MW oxy-natural gas burner (OXYFLAM-2A) from the OXYFLAME project:



# Gray Spectral Model, $z = 1.42$ m

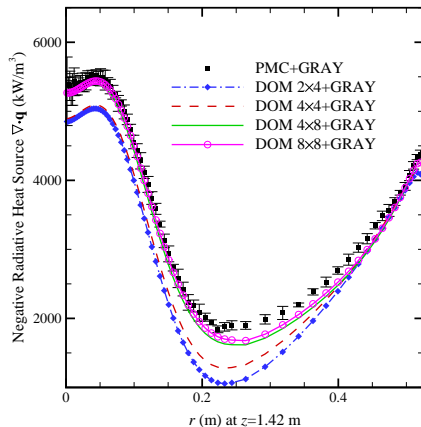
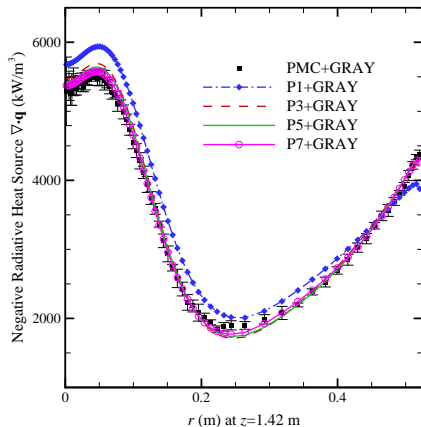
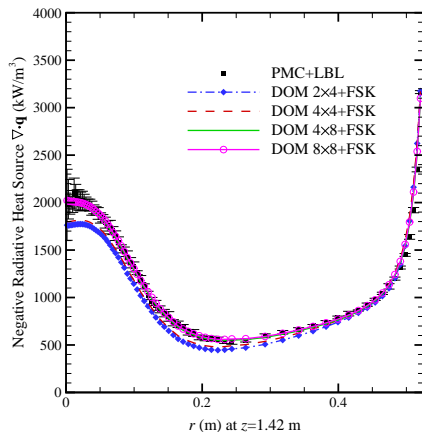
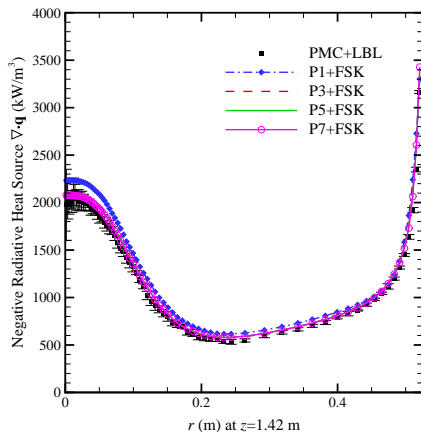


Table : Comparison of CPU time (s) of the RTE solvers for the gray case

	P <sub>1</sub>	P <sub>3</sub>	P <sub>5</sub>	P <sub>7</sub>	DOM <sub>2x4</sub>	DOM <sub>4x4</sub>	DOM <sub>4x8</sub>	DOM <sub>8x8</sub>	PMC
Gray	0.22	2.95	10.2	27.8	4.53	5.45	6.66	13.9	223 (1M×10)

# FSK Spectral Model, $z = 1.42$ m



**Table :** Comparison of CPU time (s) of the RTE solvers for the nongray case

	P <sub>1</sub>	P <sub>3</sub>	P <sub>5</sub>	P <sub>7</sub>	DOM <sub>2x4</sub>	DOM <sub>4x4</sub>	DOM <sub>4x8</sub>	DOM <sub>8x8</sub>	PMC
Nongray	0.95	12.8	49.7	111	13.1	25.8	39.4	77.5	1672 (10M×10)

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## RADIATIVE EQUILIBRIUM IN A RECTANGULAR ENCLOSURE BOUNDED BY GRAY WALLS

MICHAEL F. MODEST\*

National Research Council, NASA-Lyndon B. Johnson Space Center, Houston, Texas 77058, U.S.A.

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